

EOS7C-ECBM: MODIFICATION OF EOS7C TO INCLUDE ENHANCED COAL-BED METHANE AND THE DUSTY GAS MODEL

Stephen W. Webb¹ and Curtis M. Oldenburg²

¹Canyon Ridge Consulting LLC
10 Canyon Ridge Dr.
Sandia Park, NM, USA, 87047
e-mail: Stephen.Webb.CRC@gmail.com

²Lawrence Berkeley National Laboratory
Earth Sciences Division 74-316C
Berkeley, CA, USA, 94720
email: cmoldenburg@lbl.gov

ABSTRACT

EOS7C is an equation of state module for the TOUGH2 program for CO₂ or N₂ in Methane (CH₄) Reservoirs. Additions have been made to the EOS7C Version 1.0 module to include Enhanced Coal Bed Methane (ECBM) modifications and the Dusty Gas Model for gas-phase diffusion.

The ECBM modifications to the EOS7C equation of state incorporate the extended Langmuir isotherm for sorbing gases, including the change in porosity associated with the sorbed gas mass. Comparison to hand calculations for pure gas and binary mixtures shows very good agreement. Application to a CO₂ well injection problem given by Law et al. (2002) shows reasonable agreement.

The Dusty Gas Model (DGM) modifications add options to calculate gas diffusion using the Dusty-Gas Model, including separate and coupled approaches. The DGM is recommended for use in lower permeability reservoirs (10⁻¹⁵ m² or less) (Oldenburg et al., 2004a). Comparison to low-permeability pure gas diffusion data shows excellent agreement. The results from the DGM are compared to the Fick's law behavior for diffusion across a capillary fringe. The differences between the models are small, due to the relatively high permeability (10⁻¹¹ m²).

INTRODUCTION

EOS7C is an equation-of-state module for TOUGH2 for CO₂ or N₂ in methane (CH₄) reservoirs. The TOUGH2 EOS7C Version 1.0 module for CO₂ (Oldenburg et al., 2004b) has been enhanced to include Enhanced Coal Bed Methane (ECBM) modifications. In addition, the Dusty Gas Model for gas-phase diffusion

(Webb, 1998) has been included. Each modification will be discussed separately. Additional details are given in Webb (2011).

Enhanced Coal Bed Modifications

In Enhanced Coal Bed Methane, CO₂ is pumped into methane-rich coal beds. Due to adsorption processes, the CO₂ is sorbed onto the coal, which displaces previously sorbed methane.

The gas storage capacity for a single gas species is given by the Langmuir relationship (Law et al., 2002)

$$G_s = G_{sL} \left[1 - (w_a + w_{we}) \right] \frac{P}{P + P_L} \quad (1)$$

where

G_s	gas storage capacity (sm ³ /kg-coal)
G_{sL}	dry, ash-free Langmuir storage capacity (sm ³ /kg-coal)
w_a	ash weight fraction
w_{we}	equilibrium moisture weight fraction
P	pressure (Pa)
P_L	Langmuir pressure (Pa)

The individual Langmuir parameters from Equation (1) are used to model multiple gas species through the extended Langmuir isotherm

$$G_{si} = G_{sLi} \left[1 - (w_a + w_{we}) \right] \frac{\frac{P y_i}{P_{Li}}}{1 + P \sum_{j=1}^{nc} \frac{y_j}{P_{Lj}}} \quad (2)$$

where

y	mole fraction of component i in the gas phase
i	component i
nc	number of components

Gas sorption is added to the basic mass balance equation in TOUGH2 as follows:

$$M_{gas}^{\kappa} = \phi \sum_{gas} S_{gas} \rho_{gas} X_{gas}^{\kappa} + (1 - \phi) \rho_{coal} G_{si} \rho_{gas,STP} \quad (3)$$

where M_{gas}^{κ} is the mass of component κ in the gas phase per unit volume and ϕ is total fluid volume fraction including the sorbed gases similar to the Zarrouk and Moore (2009) modifications. The sorbed gases lead to coal-bed volume changes.

In order to include coal-bed shrinking and swelling, the sorbed gases change the local porosity as determined by the sorbed gas density and the amount of gas sorbed. Two porosities or volumes are defined: (1) the total fluid porosity (volume), which includes any sorbed gas volume; and (2) the net fluid porosity (volume), which is the net value available for fluids. These terms are shown schematically in Figure 1.

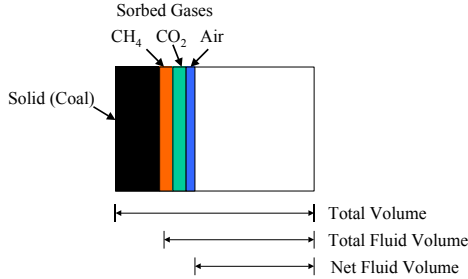


Figure 1. Volume nomenclature

$$\begin{aligned} - \left[\frac{1}{D_1^{K*}} + \frac{y_2}{D_{12}^*} + \frac{y_3}{D_{13}^*} \right] N_1^{D,g} + \frac{y_1}{D_{12}^*} N_2^{D,g} + \frac{y_1}{D_{13}^*} N_3^{D,g} &= \frac{\nabla P_1}{RT} = \frac{P \nabla y_1}{RT} + \frac{y_1 \nabla P}{RT} \\ \frac{y_2}{D_{21}^*} N_1^{D,g} - \left[\frac{y_1}{D_{21}^*} + \frac{1}{D_2^{K*}} + \frac{y_3}{D_{23}^*} \right] N_2^{D,g} + \frac{y_{21}}{D_{23}^*} N_3^{D,g} &= \frac{\nabla P_2}{RT} = \frac{P \nabla y_2}{RT} + \frac{y_2 \nabla P}{RT} \\ \frac{y_3}{D_{31}^*} N_1^{D,g} + \frac{y_3}{D_{32}^*} N_2^{D,g} - \left[\frac{y_1}{D_{31}^*} + \frac{y_2}{D_{32}^*} + \frac{1}{D_3^{K*}} \right] N_3^{D,g} &= \frac{\nabla P_3}{RT} = \frac{P \nabla y_3}{RT} + \frac{y_3 \nabla P}{RT} \end{aligned} \quad (5)$$

where the two terms on the right-hand side represent ordinary and Knudsen diffusion driving forces, respectively. Note that self diffusion, D_{11}^* , is not explicitly included in the equation set.

For a single component, the DGM equation reduces to

$$N_1^{D,g} = -D_1^{K*} \frac{\nabla P_1}{RT} \quad (6)$$

Dusty Gas Model

The general form of the Dusty Gas Model for the gas diffusion of component i is given by (Thorstenson and Pollack, 1989)

$$\sum_{j=1, j \neq i}^n \frac{y_i N_j^D - y_j N_i^D}{D_{ij}^*} - \frac{N_i^D}{D_i^{K*}} = \frac{(\nabla P_i - \rho_g g)}{RT} \quad (4)$$

where N^D is the molar diffusive flux, y is the gas-phase mole fraction, D_{ij}^* is the effective binary diffusion coefficient, D^{K*} is the effective Knudsen diffusion coefficient, P is the pressure, R is the gas constant, and T is the temperature. The summation for component j is over all components in the system except i , such that the diffusion of all gas components is coupled.

For a three-component system and ignoring gravity for simplicity in this presentation, the set of equations becomes

where the Knudsen diffusion coefficient models the “slip” of the gas, or the Klinkenberg effect.

As can be seen from Equation (5), the diffusion of any single component may be strongly coupled with the diffusion of the other components. Therefore, in general, a single equation for the diffusion of a given component cannot be developed. Two exceptions are binary gas diffusion, where equations can be developed as given by Thorstenson and Pollock (1989), and

trace gas diffusion, where an effective tortuosity can be defined for use with Fick's law (Webb and Pruess, 2003) that will give the same results as the DGM.

For diffusion of dissolved components in the liquid phase, a simple Fick's law model has been used. The model is different from that of Pruess et al. (1999), however, in that Fick's law is based on mole fractions rather than mass fractions. The present model gives equimolar diffusive fluxes in the liquid, while the model used by Pruess et al. (1999) gives equal and opposite mass fluxes. The diffusive fluxes for each dissolved component (including water) are given by

$$N_i^{D,\ell} = -D_{li,\ell}^* c_\ell \nabla x_i \quad (7)$$

where i applies to all the components including water.

2.2.1 Coupling of Diffusive Fluxes

The above equations predict gas and liquid diffusion for uniform properties under single-phase conditions. For non-uniform properties and multiphase conditions, the solution of the above equations becomes much more

complicated. Pruess and Webb (1999) developed a multiphase diffusion scheme by invoking conservation of total flux across the interface, which leads to harmonic weighting of the strength coefficient. However, their diffusion equations were based on Fick's law, such that coupling between components in a given phase was not included. Only the coupling of gas and liquid diffusion was considered.

The general concept of a weighting scheme for diffusion is that the fluxes to and from an "interface" condition are equal. This "interface" condition is defined by the equality of fluxes. For simple cases, harmonic weighting is the appropriate weighting scheme as discussed by Tsang and Pruess (1990). The same principle of conservation of mass flux, or diffusive flux, will be used in this case, based on the combined gas and liquid diffusive fluxes.

As discussed by Pruess and Webb (1999), the weighting scheme must consider the combined fluxes rather than each one individually. For example, the DGM equation for component 1 can be written in terms of the unspecified interface conditions (mole fraction and pressure) as follows

$$-\left[\frac{1}{D_1^{K*}} + \frac{y_2}{D_{12}^*} + \frac{y_3}{D_{13}^*}\right] N_1^{D,g} + \frac{y_1}{D_{12}^*} N_2^{D,g} + \frac{y_1}{D_{13}^*} N_3^{D,g} = \frac{P}{RT} \frac{y_{1,i} - y_{1,u}}{d_u} + \frac{y_1}{RT} \frac{P_i - P_u}{d_u} \quad (8)$$

where subscript i denotes the interface condition, and d_u is the distance from gridblock 1 to the interface, or the upstream length. Naturally, the properties of gridblock 1 are used for the coefficients. Similarly, the downstream equation is

$$-\left[\frac{1}{D_1^{K*}} + \frac{y_2}{D_{12}^*} + \frac{y_3}{D_{13}^*}\right] N_1^{D,g} + \frac{y_1}{D_{12}^*} N_2^{D,g} + \frac{y_1}{D_{13}^*} N_3^{D,g} = \frac{P}{RT} \frac{y_{1,d} - y_{1,i}}{d_d} + \frac{y_1}{RT} \frac{P_d - P_i}{d_d} \quad (9)$$

and the properties of gridblock 2 are used. Similar sets of equations can be written for each gas-phase component and each liquid-phase component.

The gas equations specify the interfacial mole fraction in terms of the gas mole fraction, while the liquid equations use the liquid mole fraction for the interface. The difference between the

mole fractions is resolved by defining an effective value of Henry's constant, which is defined as

$$K_{H,i,eff} = K_{H,i} \frac{c_\ell}{c_g} = \frac{y_{g,i}}{x_{\ell,i}} \quad (10)$$

so the liquid interfacial mole fractions can be converted to gas interfacial mole fractions.

$K_{H,i,eff}$ for the interface is calculated from the upstream and downstream gridblocks based on the element mole fractions. Only gridblocks with gas and liquid in them are considered. The value at the interface is estimated by harmonic weighting of the gridblock values.

The values of the interfacial mole fractions and total interfacial pressure are calculated by invoking equal upstream and downstream total molar fluxes (gas plus liquid) to and from the interface for each component, as well as the requirement that the mole fractions sum to 1.0.

Therefore, for a three-component system, there are 16 equations and 16 unknowns. For a five-component system such as in EOS7C, there are 26 equations and 26 unknowns for the fully coupled solution.

Verification of Modifications

ECBM

Verification of the modifications to TOUGH2 for the ECBM is provided through comparison of the output from the code to literature results. The first verification exercise compares the results from extended Langmuir isotherm calculations with the results presented by Arri et al. (1992). These results are for pure gas and binary gas sorption, where the extended Langmuir parameters are specified by Arri et al. (1992). The second verification exercise is for a sample problem presented by Law et al. (2002), which has been used for comparison of various ECBM simulators.

Isotherms

Arri et al. (1992) present the results of isotherm calculations for pure gas and binary gas conditions for CH₄, CO₂, and N₂. The results from the present calculation are presented in the same English units used in the original reference for ease of comparison. Figure 2 shows the pure gas isotherm results; the extended Langmuir values are summarized in Table 1. The solid line is the isotherm given earlier by Equation (1) with zero ash and moisture weight fractions, while the symbols are the results from the

modified TOUGH2 code. The agreement is excellent.

Table 1. Langmuir Parameters (Arri et al., 1992)

Gas	G _{SL} (SCF/ton)	p _L (psia)
CO ₂	1128	204.5
CH ₄	759	362.3
N ₂	616	1458.

Figure 3 presents results for binary gas adsorption using the extended Langmuir isotherm constants given in Table 1. The plot shows the CH₄-N₂ binary gas sorption isotherms at 500 psia given by Equation (2) and the results calculated with the modified TOUGH2 program given by the symbols. The agreement is excellent.

The species splits in the gas phase and the sorbed phase are shown in Figure 4 for the mixture given above. These curves are independent of pressure because pressure is completely defined by the pure gas Langmuir isotherms, as discussed by Arri et al. (1992). The separation factor, α , is given by

$$\alpha_i = \frac{\left(\frac{x}{y}\right)_i}{\left(\frac{x}{y}\right)_j} \quad (11)$$

where x is the sorbed phase mole fraction and y is the gas phase mole fraction, and i and j are the two gases. The value of the separation factor can be calculated from (Arri, et al., 1992)

$$\alpha_i = \frac{(G_{sL} / p_L)_i}{(G_{sL} / p_L)_j} \quad (12)$$

which is not a function of pressure. For a binary gas mixture, equation (11) can be rearranged to give the gas phase mole fraction of component i as

$$y_i = \left(1 + \alpha_i \frac{1 - x_i}{x_i}\right)^{-1} \quad (13)$$

which is the solid line in the figures. Again, the agreement between the results from the modified TOUGH2 code and the above equation is excellent.

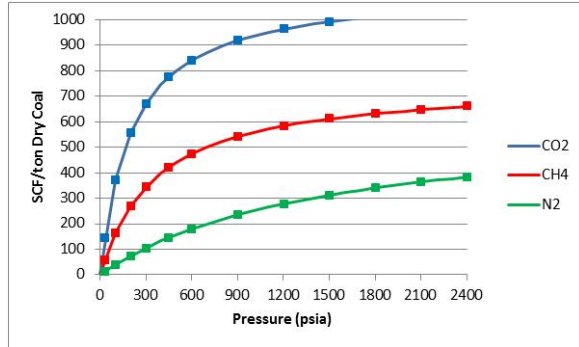


Figure 2. Pure gas isotherms

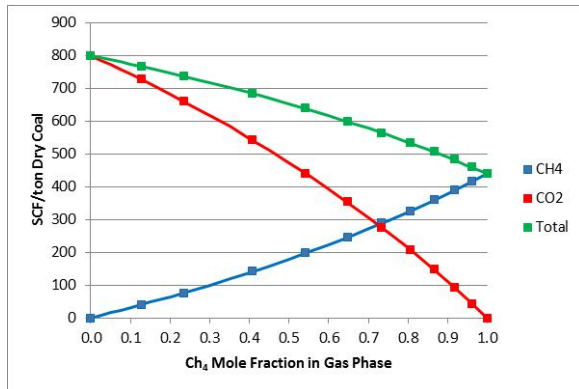


Figure 3. CH₄-CO₂ sorption at 500 psia

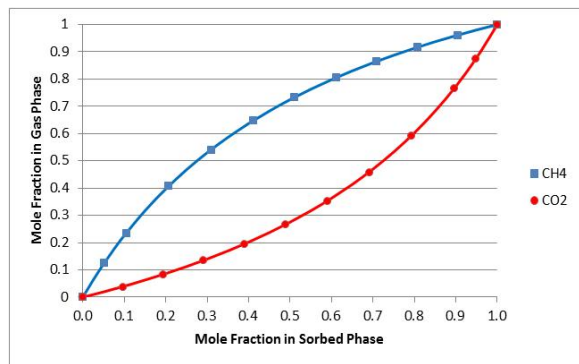


Figure 4. CH₄-CO₂ splits at 500 psia

Law et al. (2002) Problem

Law et al. (2002) have presented a comparison of ECBM simulators for two simplified problem sets. The first problem is a single-well CO₂ injection test, while the second problem is a five-spot CO₂-ECBM recovery process. The

geometry and relative permeability functions are explicitly defined by Law et al. (2002); note that there is no capillary pressure. The first problem (single-well CO₂ injection) will be analyzed with the modified TOUGH2 code in this section.

The problem involves injecting pure CO₂ into a coal seam. Flow occurs in natural fractures that have a small natural porosity of 0.001 and a permeability of 3.65 millidarcies. The initial conditions of the reservoir are 7650 kPa, 45°C, and a gas saturation of 0.408 of pure CH₄. Coal matrix swelling/shrinkage is neglected. The problem chronology is an initial 15 days of CO₂ injection followed by a 45-day shut-in period, a 60-day production period, and a 62.5-day shut-in period. As mentioned above, no coal swelling or shrinking is included in the problem definition. This behavior is modeled by specifying the sorbed gas density as artificially high (10^{10} kg/m³) in order to effectively disable the effect of sorbed gases on the porosity.

One of the parameters from the various codes that is compared in Law et al. (2002) is the initial gas-in-place for the CH₄. The values for the five codes range from 6.0315×10^7 to 6.1681×10^7 sm³. The present code predicts 6.146×10^7 sm³.

The predicted bottom-hole pressure as a function of time is shown in Figure 5. The general behavior compares well to the results presented by Law et al. (2002) except that the borehole pressure during CO₂ injection is slightly low. This difference may be due to the treatment of the borehole, which was treated explicitly in the present simulations, or due to differences in CO₂ properties.

Figure 6 gives the gas production rate results. The flow rates of CH₄ and CO₂ are initially in agreement with the results given in Law et al. (2002). At about 64 days, however, the gas production predicted by the present code drops significantly when a gridblock near the borehole changes from pure gas to two-phase conditions and the gas relative permeability decreases from 1.0 to 0.49. This decrease in gas production rate is not seen in the results presented by Law et al. (2002). Overall, the agreement is reasonable.

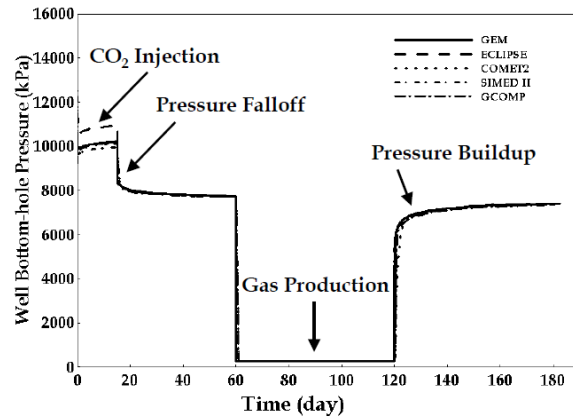


Figure 5a. Law et al. (2002) Borehole pressure results

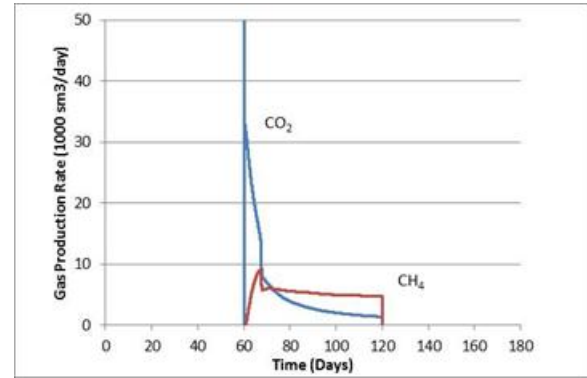


Figure 6b. Modified TOUGH2 gas production rate results

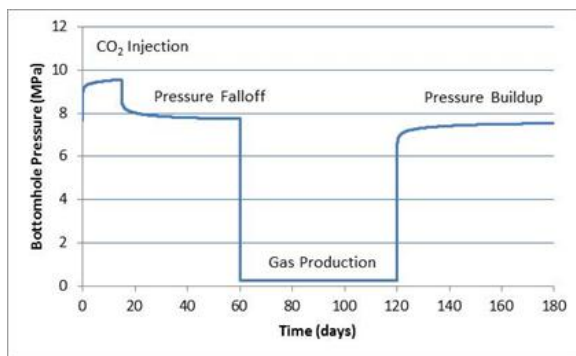


Figure 5b. Modified TOUGH2 borehole pressure results

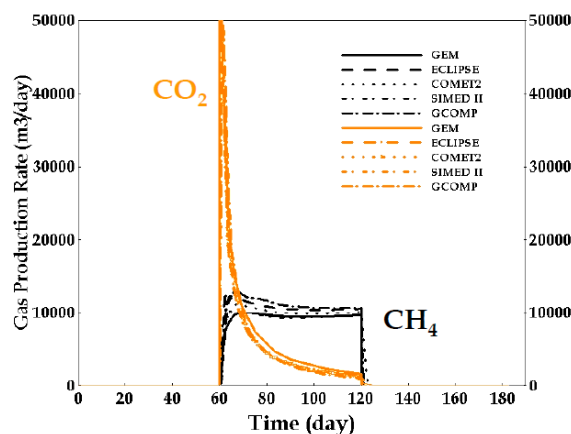


Figure 6a. Law et al. (2002) gas production rate results

DGM

In this section, the DGM is compared to the experimental data of Evans et al. (1962, 1963) for a low-permeability ($2.13 \times 10^{-18} \text{ m}^2$) graphite. The experimental data are for Argon and Helium under combined advection and diffusion conditions. Webb (1998) showed that the DGM compares well to the data, while Fick's law does not.

For this case, Mason et al. (1967) performed an integration of the DGM assuming a linear variation for the mole fraction as above. Iteration is required to obtain the desired fluxes. The experimental data compare very well to the integrated equation. Explicit equations describing the various curves were not presented, so the curves were extracted from the original figures of Mason and Malinauskas (1983). Comparison of the present modified version of TOUGH2 to these curves is given in Figure 7. The predictions compare very well to the original curves. Because the curves assume a linear mole fraction variation in their derivation, the agreement is not expected to be perfect.

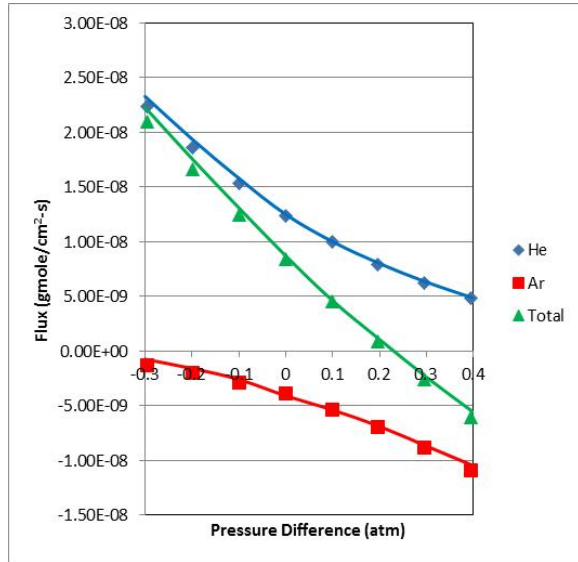


Figure 7. DGM data-model comparison for combined He-Ar advection and diffusion across low-permeability graphite

Diffusion Across a Capillary Fringe

Pruess et al. (1999) presented a sample problem involving TCE and PCE diffusion across a capillary fringe. The problem consists of TCE and PCE in the gas phase at the solubility limits above the water table, which diffuses through the capillary fringe into the water table below. The original TOUGH2 results in Pruess et al. (1999) show considerable differences between the separate and coupled diffusion models. The calculation has been redone with the modified code using the Fick's law model in TOUGH2 as well as the DGM.

Figures 8 and 9 show the results for the original Fick's law approach and for the DGM. The differences between the results are minimal. As discussed by Webb (1998) and Webb and Pruess (2003), differences between Fick's law and the DGM are minimal at higher permeabilities ($> 10^{-13} \text{ m}^2$) but they may increase to be orders of magnitude at lower values ($\sim 10^{-18} \text{ m}^2$). Therefore, the present problem is not a definitive test of the possible differences between Fick's law and the DGM.

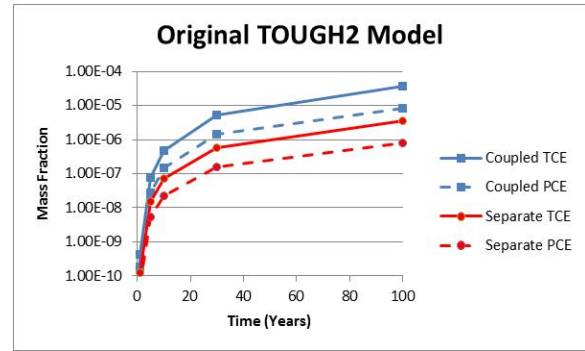


Figure 8. Separate and coupled diffusion across capillary fringe using Fick's law

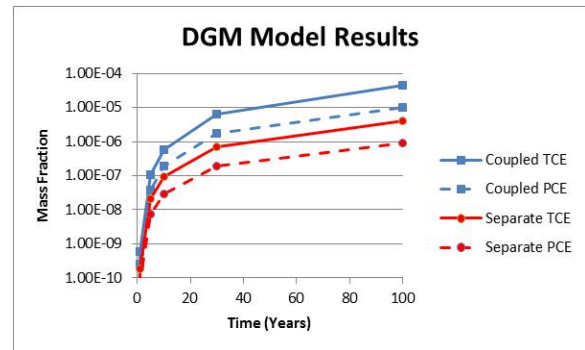


Figure 9. Separate and coupled diffusion across capillary fringe using DGM

SUMMARY AND DISCUSSION

ECBM code modifications have been successfully made to the TOUGH2-EOS7C code as demonstrated by the successful simulation of the Law et al. (2002) problem set 1. While the behavior is qualitatively similar to the behavior seen in Law et al. (2002), there are some quantitative differences, so the overall agreement is only reasonable. Further investigation of the cause for these differences is needed.

The present version of the code includes the porosity change from ECBM. Additional modifications should be made to change the permeability and connection flow area based on the change in porosity. Changes to the connection flow area could be simply related to the porosity change based on an assumed flow geometry.

Implementation of the DGM compares very well to existing gas-phase diffusion data. The use of the DGM may be limited because the computer

time increases significantly compared to the default Fick's law approach. For the Law et al. (2002) problem, the computer time increased by about a factor of three when the DGM model was used compared to the Fick's law approach. The simulation results for the DGM and Fick's law approach are not significantly different, because the permeability (3.65 millidarcies) is not that low. Improving the computational efficiency may be necessary before the DGM is used for large-scale problems.

ACKNOWLEDGMENT

This work was carried out through Lawrence Berkeley National Laboratory as part of the ZERT project, funded by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Coal Fuels, National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

REFERENCES

- Arri, L.E., D. Yee, W.D. Morgan, and M.W. Jeansonne, 1992, "Modeling Coalbed Methane Production With Binary Gas Sorption," SPE 24363, SPE Rocky Mountain Regional meeting, Casper, Wyoming, May 18-21, 1992.
- Evans, R.B., III, G.M. Watson, and J. Truitt, 1962, "Interdiffusion of gases in a low permeability graphite at uniform pressure," *J. Appl. Phys.*, 33:2682-2688.
- Evans, R.B., III, G.M. Watson, and J. Truitt, 1963, "Interdiffusion of gases in a low permeability graphite. II. Influence of pressure gradients," *J. Appl. Phys.*, 34:2020-2026.
- Law, D. H.-S., L.G.H. van der Meer, and W.D. Gunter, 2002, "Numerical Simulator Comparison Study for Enhanced Coalbed Methane Recovery Processes, Part 1: Pure Carbon Dioxide Injection, SPE 75669, SPE Gas Technology Symposium, Calgary, Alberta, 30 April – 2 May 2002.
- Mason, E.A., and A.P. Malinauskas, 1983, Gas transport in porous media: the dusty-gas model, Chem. Eng. Monograph 17, Elsevier, New York.
- Mason, E.A., A.P. Malinauskas, and R.B. Evans, III, 1967, "Flow and Diffusion of Gases in Porous Media," *J. Chemical. Physics*, 46:3199-3216.
- Oldenburg, C.M., S.W. Webb, K. Pruess, and G.J. Moridis, 2004a, "Mixing of Stably Stratified Gases in Subsurface Reservoirs: A Comparison of Diffusion Models," *Transport in Porous Media*, 54:323-334.
- Oldenburg, C.M., G.J. Moridis, N. Spycher, and K. Pruess, 2004b, "EOS7C Version 1.0: TOUGH2 Module for Carbon Dioxide or Nitrogen in Natural Gas (Methane) Reservoirs," LBNL-56589, Lawrence Berkeley National Laboratory, Berkeley, CA.
- Pruess, K., C.M. Oldenburg, and G. Moridis, 1999, "TOUGH2 User's Guide, Version 2.0," LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, CA.
- Pruess, K., and S.W. Webb, 1999, "On Finite Difference Modeling of Diffusion of Phase-Partitioning Species under Multiphase Conditions," AGU Fall Meeting, Supplement to Eos, Transactions, AGU Volume 8, Number 46, pg. F385.
- Thorstenson, D.D., and D.W. Pollock, 1989, "Gas transport in unsaturated zones: multi-component systems and the adequacy of Fick's laws," *Water Resour. Res.*, 25:477-507.
- Tsang, Y.W., and K. Pruess, 1990, "Further Modeling Studies of Gas Movement and Moisture Migration at Yucca Mountain, Nevada," LBL-29127, Lawrence Berkeley Laboratory, Berkeley, CA.
- Webb, S.W., 1998, "Gas-Phase Diffusion in Porous Media – Evaluation of an Advective-Dispersive Formulation and the Dusty-Gas Model for Binary Mixtures," *J. Porous Media*, 1:187-199.
- Webb, S.W., and K. Pruess, 2003, "The use of Fick's Law for modeling trace gas diffusion in porous media," *Transport in Porous Media*, 51:327-341.
- Webb, S.W., 2011, "EOS7C-ECBM Version 1.0: Additions for Enhanced Coal Bed Methane Including the Dusty Gas Model," Canyon Ridge Consulting Report CRC2011-0002, December 6, 2011.
- Zarrouk, S.J., and T.A. Moore, 2009, "Preliminary reservoir model of enhanced coalbed methane (ECBM) in a subbituminous coal seam, Huntly Coalfield, New Zealand. *Int. J. of Coal Geology*, 77:153-161.